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Predict First: flux-driven multi-channel integrated modelling over multiple confinement times with the gyrokinetic turbulent transport model QuaLiKiz

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An accurate and predictive model for turbulent transport fluxes driven by microinstabilities is a vital component of first-principle-based tokamak plasma simulation. However, tokamak scenario prediction over energy confinement timescales is not routinely feasible by direct numerical simulation with nonlinear gyrokinetic codes. Reduced order modelling with quasilinear turbulent transport models provides significant computational speedup, and is justified in many regimes. The justification of the quasilinear approximation for transport driving spatial scales is a consequence of the underlying structure of tokamak microturbulence, and is validated by comparison to nonlinear simulations. This approach has emerged as a successful tool for prediction of core tokamak plasma profiles. We focus on significant progress in the quasilinear gyrokinetic transport model QuaLiKiz [1,2], and its application within flux driven integrated tokamak simulation suites.

To model 1s of JET plasma on order of 24 hours with 10 CPUs, QuaLiKiz employs an approximated solution of the mode structures to significantly speed up the computation time compared to full linear gyrokinetic solvers. Additional approximations include maintaining shifted-circle $(\hat{s} - \alpha)$ geometry, and the electrostatic limit. These approximations, together with optimisation of the dispersion relation solution algorithm within integrated modelling applications, leads to flux calculations 10^{6-7} faster than local nonlinear gyrokinetic simulations. This allows tractable simulation of flux-driven dynamic profile evolution over multiple confinement times including all transport channels: ion and electron heat, main particles, impurities, and momentum. QuaLiKiz is open source and available at www.qualikiz.com.

In this contribution, we will summarize the justification of the quasilinear approximation [3,4], sketch the basis of the QuaLiKiz transport model and its validity in comparison to nonlinear simulations, and illustrate validation of the model against experimental measurements at JET through flux-driven simulations within the JINTRAC integrated modelling suite [5,6], see figure 1 for an example. This capability 1) enhances the interpretation of present-day experiments, 2) enables "Predict First" simulations to aid with experimental optimization, and 3) allows theory-based extrapolation to future machine performance, at least with respect to core turbulence physics. While we focus here on JINTRAC simulations, QuaLiKiz is also coupled to the ASTRA [7,8], CRONOS [9] and ETS [10] integrated modelling codes.

Recent QuaLiKiz applications within integrated modelling include: W-accumulation interpretation and optimization, where the QuaLiKiz prediction of background kinetic profiles is critical for setting the neoclassical heavy impurity transport level [11-13]; modelling of multiple-isotope experiments at JET, where fast isotope mixing in the Ion Temperature Gradient (ITG) regime is crucial for experimental interpretation and has important implications for potential scenarios in JET DT, as well as for reactor burn control [14]; development of Uncertainty Quantification methods using Gaussian Process Regression to enhance statistical rigour in model validation, providing avenues for error propagation within QuaLiKiz simulations in integrated modelling [15]; predictive modelling for ITER scenarios, which predict the target Q~10 when using a theory-based pedestal boundary condition [16]; and predictive modelling for DTT scenarios [17].

Beyond standard application within integrated modelling, QuaLiKiz has been leveraged for the development of realtime calculation capability for scenario optimization and realtime-oriented applications. This is based on machine learning methods, where a large database of pre-calculated QuaLiKiz runs is used to train feedforward neural networks to accurately reproduce model predictions. The neural network transport model provides a further 6 orders of magnitude speedup, 1 trillion times faster than the anchoring nonlinear simulations [18]. By coupling to the RAPTOR [19] control-oriented fast tokamak simulator, realtime-capable transport predictions are possible. This opens up a plethora of possibilities and innovation in realtime controller design and validation, scenario preparation, and discharge optimization.

While QuaLiKiz has had significant predictive success, continuously challenging and improving the model is a crucial component for instilling validity in wide parameter space. Beyond its role in experimental interpretation and prediction, reduced models such as QuaLiKiz are a key player in the multi-fidelity model hierarchy due to its feasibility for systematic comparison with experiments and identifying trends in model validation. This spurs further research, also incorporating higher fidelity linear and nonlinear models, ultimately improving our understanding of core tokamak turbulence physics. We thus conclude with an overview of recent work dedicated to testing and improving the underlying Qua-LiKiz assumptions. This includes: modification of the collisionality model, critical for obtaining the correct parameter dependencies of Trapped Electron Modes (TEM); validating the QuaLiKiz Electron Temperature Gradient (ETG) model versus multi-scale nonlinear GENE simulations; testing validity of QuaLiKiz towards the L-mode edge, where the standard ITG/TEM/ETG paradigm breaks down at high collisionality, due to the onset of modes with a drift-resistive nature, currently out of QuaLiKiz scope; testing the impact of $s-\alpha$ geometry on the turbulence regime, compared to full geometry, particularly at more outer radii where shaping effects are more prominent. Future work will extend QuaLiKiz to electromagnetic regimes.

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